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Molecular recognition of organic vapors by adamantylcalix[4]arene in QCM sensor using partial binding reversibility

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Abstract

The parameters of stability, guest binding reversibility, and Gibbs energy of guest inclusion were determined for clathrates of adamantylcalix[4]arene (1), These data provide a new insight into the structure-property relationships in vapor sensor applications of clathrate-forming hosts. A thin layer of 1, used in the quartz mierobalance (QCM) sensor, demonstrates a selectivity for organic vapors, which depends on the regeneration technique after the guest binding. Complete regeneration of 1 on the sensor surface was reached through the exchange of bound guest with ethanol vapor, which forms an unstable clathrate with 1. The efficiency of the used regeneration technique was proved by comparing the QCM data with the isotherms of guest vapor sorption by guest-free host 1 and with the data of simultaneous thermogravimetry and differential scanning calorimetry for the saturated clathrates of 1. In sensor, the extent of host regeneration without guest exchange depends on the guest molecular structure. This extent, or guest-binding reversibility parameter, being determined in a combination with the sensor responses of completely regenerated 1 to guest vapors, increases the recognition capability of single sensor device. Using this technique, 13 of 15 studied guests were discriminated. The structural hints on the suitable sensor properties of 1 were found in the determined X-ray monocrystal data for clathrate of this host with toluene. © 2008 American Chemical Society.

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